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# Configuration interaction applied to resonant states in semiconductors and semiconductor nanostructures

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**Abstract.** A new approach for calculation of resonant state parameters is developed. The method proposed allows to solve different scattering problems, such as scattering and capture probability as well as calculations of shifts and widths of energy levels. It has been applied to the problem of resonant states induced by impurities in the barrier of quantum wells and by strain in uniaxially stressed germanium.

## Introduction

Quasistationary (or resonant) states have been studied in atomic physics very well. Semiconductors are other systems where resonant states play a significant role in physical processes. Such states appear, for example, in gapless semiconductors when doped by shallow acceptors. The system of special interest is uniaxially strained germanium where the generation of THz radiation has been achieved [1, 2].

Here we suggest a new method for calculating the parameters of resonant states and the probability of resonant scattering, capture and emission of carriers. The approuch is based on the configuration interaction method which was first introduced by Fano [3] in the problem of autoionization of He. The main idea is to choose two different hamiltonians for the initial approximation one for continuum states and the other for localized states. The method is applied to resonant states induced (i) by impurities in the barrier of quantum wells and (ii) by shallow acceptors in Ge under stress.

## 1. Resonant states induced by localized states in barriers

We will demonstrate the general idea by applying it to the system consisting of a quantum well (QW) and one impurity in the barrier. The full hamiltonian is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(z) + V_d(\mathbf{r} - \mathbf{r}_0), \qquad (1)$$

where the potential of the QW $V(z)$ is shown in Fig. 1, $V_d$ is the defect potential and $\mathbf{r}_0 = (0, 0, z_0)$ is the position of defect.

As an initial approximation for the wave function of the localized state induced by the impurity we use the solution of the equation:

$$\left[-\frac{\hbar^2}{2m}\Delta + V_d(\mathbf{r} - \mathbf{r}_0)\right]\varphi(\mathbf{r} - \mathbf{r}_0) = E_0\varphi(\mathbf{r} - \mathbf{r}_0). \qquad (2)$$

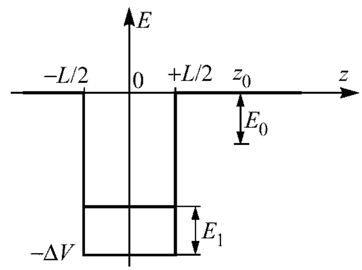


**Fig. 1.** The parameters of the well and impurity.

The wave functions of continuum states $\psi_{\mathbf{k}}(\mathbf{r})$ satisfy the following equation:

$$\left[-\frac{\hbar^2}{2m}\Delta + V(z)\right]\psi_{\mathbf{k}}(\mathbf{r}) = E_k\psi_{\mathbf{k}}(\mathbf{r}). \tag{3}$$

We are considering a QW with one energy level only, so that

$$E_k = -\Delta V + E_1 + \varepsilon_k, \tag{4}$$

where $E_1$ is the space quantization level and $\varepsilon_k = \hbar^2k^2/2m$ is kinetic energy of the 2D motion. So we can write for $\psi_{\mathbf{k}}(\mathbf{r})$:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{S}}\phi(z)e^{i\mathbf{k}\rho}, \tag{5}$$

where $S$ is a normalizing square.

Now we consider the problem of scattering of the in-plane moving carrier by the impurity in the barrier. Following Dirac, we construct the wave function in terms of scattering theory in the following form:

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}(\mathbf{r}) + a_{\mathbf{k}}\varphi(\mathbf{r}-\mathbf{r}_0) + \sum_{\mathbf{k}'}\frac{t_{\mathbf{kk}'}}{\varepsilon_k - \varepsilon_{k'} + i\gamma}\psi_{\mathbf{k}'}(\mathbf{r}), \quad \gamma \to 0. \tag{6}$$

As the presence of one impurity does not perturb the continuum spectrum significantly, $\Psi_{\mathbf{k}}(\mathbf{r})$ should correspond to the energy $E_k$. Solving the Schrödinger equation with the full hamiltonian (1) for $\Psi_{\mathbf{k}}(\mathbf{r})$ one obtains the following expressions for $a_{\mathbf{k}}$ and $t_{\mathbf{kk}'}$:

$$a_{\mathbf{k}} = \frac{1}{\sqrt{S}}\frac{V_{\mathbf{k}}}{E_k - (E_0+\Delta E) + i\Gamma/2}, \quad t_{\mathbf{kk}'} = \frac{1}{S}\frac{V_{\mathbf{k}}Z^*_{\mathbf{k}'}}{E_k - (E_0+\Delta E) + i\Gamma/2} \tag{7}$$

The energy shift $\Delta E$ and the width $\Gamma/2$ of the resonant level are given by:

$$\Delta E = \delta - \frac{1}{(2\pi)^2}\int d^2k' Z^*_{\mathbf{k}'}W_{\mathbf{k}'} + \frac{1}{(2\pi)^2}P\int d^2k'\frac{Z^*_{\mathbf{k}'}V_{\mathbf{k}'}}{E_k - E_{k'}}, \tag{8}$$

$$\frac{\Gamma}{2} = \frac{1}{4\pi}\int d^2k' Z^*_{\mathbf{k}'}V_{\mathbf{k}'}\delta(E_k - E_{k'}). \tag{9}$$

Here the matrix elements

$$V_{\mathbf{k}} = \sqrt{S}\langle\varphi|V_d|\psi_{\mathbf{k}}\rangle,\ W_{\mathbf{k}} = \sqrt{S}\langle\varphi|\psi_{\mathbf{k}}\rangle,\ \delta = \langle\varphi|V(z)|\varphi\rangle,\ Z_{\mathbf{k}} = \sqrt{S}\langle\varphi|V(z)|\psi_{\mathbf{k}}\rangle, \tag{10}$$

are introduced.

The probability of resonant elastic scattering $W_{\mathbf{kk}'}$ of 2D carriers and the capture probability $W_{\mathbf{k}r}$ are given by:

$$W_{\mathbf{kk}'} = \frac{2\pi}{\hbar}|t_{\mathbf{kk}'}|^2\delta(\varepsilon_k - \varepsilon_{k'}), \qquad W_{\mathbf{k}r} = |a_{\mathbf{k}}|^2, \tag{11}$$

respectively. Both probabilities contain the same resonant denominator.

The resonant scattering should be introduced into the kinetic equation when one solves the problem of the 2D carriers distribution function under an electric field applied in plane of the quantum well. This scattering affects the distribution function $f_{\mathbf{k}}$ of hot carriers, which is connected with the population of impurities in the barrier $f_r$ [4]:

$$f_r = \sum_{\mathbf{k}} W_{\mathbf{k}r} f_{\mathbf{k}}. \tag{12}$$

## 2. Resonant acceptor states in uniaxially strained germanium

Tetraherally coordinated semiconductors (eg. GaAs, Ge, Si) have a fourfold degenerate top of the valence band. When strained, the top of valence band is split into two doubly degenerate states. The ground state of an acceptor shows the same behavior under uniaxial stress. At some critical value of the stress — when the splitting is larger than the acceptor binding energy — one of the split levels is shifted into the continuous spectrum of the other valence subband and becomes resonant. An effective optical transitions between resonant and localized states of the same impurities can take place. If the electric field is strong enough an electric impurity breackdown occurs and practically all localized impurity states become depopulated. Now capture and emission processes lead to an effective population of resonant states. This may cause an intracenter population inversion that is the basis for THz generation [1, 2].

Resonant acceptor states were considered in [4] by using the Dirac approach, which requires choosing an initial approximation hamiltonian giving localized states overlapping with the continuous spectrum. The approach in [4] applies for large stresses and for small quasimomenta but it fails for the region of the spectrum where resonant states are present.

Using our new approach we will consider the ground resonant state induced by shallow acceptors in uniaxially strained p-Ge along [001] direction.

As the initial approximation for localized states we choose the diagonal part of the Luttinger hamiltonian and the Coulomb potential of an acceptor. For continuum states we use the eigenfunctions $\psi_{\mathbf{k}}^{\pm 1/2}(\mathbf{r})$ of the full Luttinger hamiltonian for free holes in cylindrical approximation. Following the procedure from the first section we are looking for wave functions in the form:

$$\begin{aligned}\Psi_{\mathbf{k}}^{\pm 1/2} &= \psi_{\mathbf{k}}^{\pm 1/2} + a_{\mathbf{k}}^{\pm 1/2,+3/2}\varphi^{+3/2}(\mathbf{r}) + a_{\mathbf{k}}^{\pm 1/2,-3/2}\varphi^{-3/2}(\mathbf{r}) \\ &+ \sum_{\mathbf{k}'} \frac{t_{\mathbf{kk}'}^{\pm 1/2,+1/2}}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'} + i\gamma}\psi_{\mathbf{k}'}^{+1/2} + \sum_{\mathbf{k}'} \frac{t_{\mathbf{kk}'}^{\pm 1/2,-1/2}}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'} + i\gamma}\psi_{\mathbf{k}'}^{-1/2}.\end{aligned} \tag{13}$$

We carried out calculations taking into account non-resonant scattering by the Coulomb potential in first order only. The probability of capturing holes with momentum projection $+1/2$ $W_{\mathbf{k}r}$ and the probability of elastic resonant scattering $W_{\mathbf{kk}'}$ are defined now by

$$W_{\mathbf{k}r} = \left|a_{\mathbf{k}}^{+1/2,+3/2}\right|^2 + \left|a_{\mathbf{k}}^{+1/2,-3/2}\right|^2. \tag{14}$$

$$W_{\mathbf{kk}'} = \frac{2\pi}{\hbar}\left(\left|t_{\mathbf{kk}'}^{+1/2,+1/2}\right|^2 + \left|t_{\mathbf{kk}'}^{+1/2,-1/2}\right|^2\right)\delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}) \tag{15}$$

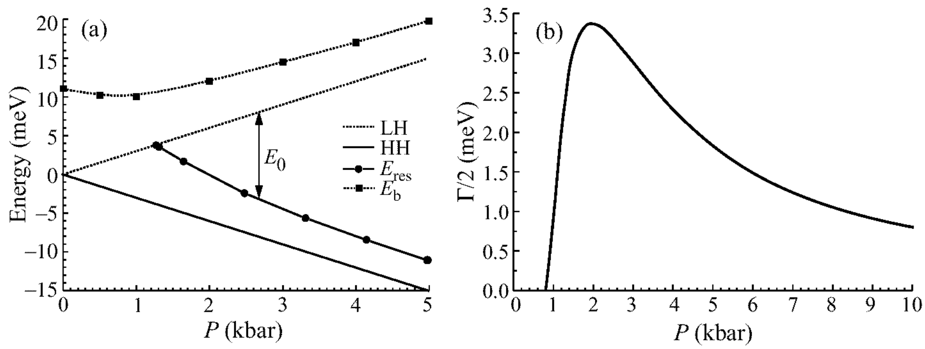


**Fig. 2.** The position (a) and width (b) of resonant state as a function of stress applied in [001] direction.

The expressions for the case of momentum projection $-1/2$ are similar. The results of calculations of the resonant level shift and level width are given in Fig. 2.

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